=>
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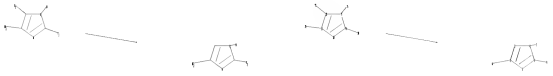


chain nodes :
6 7 9 15 16 17 19
ring nodes :
1 2 3 4 5 10 11 12 13 14
chain bonds :
2-6 4-7 5-9 11-16 12-17 13-15 14-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 10-11 10-14 11-12 12-13 13-14
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-9 10-11 10-14 11-12 12-13 12-17 13-14 14-19
exact bonds :
2-6 4-7 11-16 13-15

G1:Cl,Br

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 19:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 10

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 14:01:28 FILE 'CASREACT'
SCREENING COMPLETE - 98 REACTIONS TO VERIFY FROM 9 DOCUMENTS

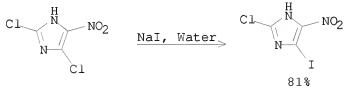
100.0% DONE 98 VERIFIED 8 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L2 1 SEA SSS FUL L1 (8 REACTIONS)

=> d l2

L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 20



REF: PCT Int. Appl., 2005077913, 25 Aug 2005
NOTE: regioselective
CON: 35 hours, 102 deg C

=> d l2 ibib abs

L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:229859 CASREACT <<LOGINID::20080920>>
TITLE: Producing 4-nitroimidazole compounds
INVENTOR(S): Shinhama, Koichi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

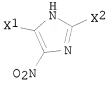
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005077913	A1	20050825	WO 2005-JP2668	20050215

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005212093	A1	20050825	AU 2005-212093	20050215
AU 2005212093	B2	20080403		
CA 2555372	A1	20050825	CA 2005-2555372	20050215
EP 1720838	A1	20061115	EP 2005-710450	20050215
EP 1720838	B1	20070704		
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1922154	A	20070228	CN 2005-80005310	20050215
AT 366241	T	20070715	AT 2005-710450	20050215
BR 2005007777	A	20070717	BR 2005-7777	20050215
ES 2289695	T3	20080201	ES 2005-710450	20050215
JP 2006117628	A	20060511	JP 2005-42010	20050218
IN 2006KN02205	A	20070525	IN 2006-KN2205	20060804
MX 2006PA09262	A	20061113	MX 2006-PA9262	20060815
US 20070161802	A1	20070712	US 2006-589864	20060817
KR 830386	B1	20080519	KR 2006-717553	20060830
PRIORITY APPLN. INFO.:			JP 2004-41381	20040218
			JP 2004-278999	20040927
			WO 2005-JP2668	20050215

OTHER SOURCE(S): MARPAT 143:229859

GI



I

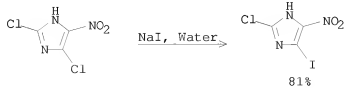
AB The present invention provides a method for producing a 4-nitroimidazole (I, X1 = H) at high yield and at high purity by a safe method causing few dangers such as explosion. The production method comprises iodinating a 4-nitroimidazole compound I (wherein each of X1 and X2 represents a Cl or Br), and then reducing the obtained I (X1 = I and X2 is the same as defined above). E.g., 2-bromo-5-iodo-4-nitroimidazole was prepared from 2,5-dibromo-4-nitroimidazole and NaI and the product treated with PtO in the presence of triethylamine in ethanol to give 2-bromo-4-nitroimidazole.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l2 1-8

L2 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 20



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